

Probabilistic positional association of astrophysical sources between catalogs

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ABSTRACT

We describe a simple probabilistic method to cross-identify astrophysical sources from different catalogs and provide the probability that a source is associated with a source from another catalog or that it has no counterpart. When the positional uncertainty in one of the catalog is unknown, this method may be used to derive its typical value and even to study its dependence on the size of objects. It may also be applied when the true centers of a source and of its counterpart at another wavelength do not coincide.

We extend this method to the case when there are only one-to-one associations between the catalogs.

Key words. Methods: statistical – Catalogs – Astrometry – Galaxies: statistics – Stars: statistics

1. Introduction

The problem of cross-identifying sources between two catalogs K and K' has previously been studied by Condon et al. (1975), de Ruiter et al. (1977), Prestage & Peacock (1983), Sutherland & Saunders (1992) and Rutledge et al. (2000), among others. As evidenced by recent papers of Budavári & Szalay (2008) and Pineau et al. (2011), this field is still very active and will be more so with the wealth of forthcoming multiwavelength data. Usually, the association is performed using a “likelihood ratio”: this quantity is typically computed as the ratio of the probability of finding, at some distance from a source $M_i \in K$, a source $M'_j \in K'$, if M'_j is a counterpart of M_i , to the probability that M'_j is a chance association at the same position, given the local surface density of K' -sources. As noticed by Sutherland & Saunders (1992), there has been some confusion in the definition and interpretation of the likelihood ratio, and, more importantly, in the estimation of the probability¹ that a source in K' is the counterpart of a source in K .

When associating sources from catalogs at different wavelengths, some authors include in this likelihood ratio some *a priori* information on the spectral energy distribution (SED) of the source. As this work began, our primary goal was to build template observational SED’s of galaxies from the optical to the far-infrared for different types of galaxies. We initially intended to cross-identify the IRAS Faint Source Survey (Moshir et al. 1992, 1993) with the LEDA database (Paturel et al. 1995). Because of the large positional inaccuracy of IRAS data, special care was needed to identify optical sources with infrared ones. While IRAS data are by now quite outdated and have been superseded by Spitzer observations, we still think that the procedure we developed at that time may be valuable for other studies. Because we aimed to fit synthetic SED’s to the template observational ones, we could not and did not want to make assumptions on the SED of sources based on their type, since this would have biased the procedure. We therefore rely in what follows only on the positions to associate sources between catalogs.

The method we use is essentially similar to that of Sutherland & Saunders (1992). Because thinking in terms of probabilities rather than of likelihood ratios highlights some implicit assumptions, we found it however useful for the sake of clarity to detail hereafter our calculations; this allows us moreover to extend our work to a case not covered by papers cited above (see Sect. 4).

We define our notations and explicit our general assumptions in Sect. 2. In Sect. 3, we compute the probability of association under the assumption that a K -source has at most one counterpart in K' but that several K -sources may have the same counterpart (“several-to-one” associations). We moreover determine the fraction of sources with a counterpart and, if unknown, estimate the uncertainty on the position in one of the catalogs. In Sect. 4, we compute the probability of association under the assumption that a K -source has at most one counterpart in K' and that no other K -source has the same counterpart (“one-to-one” associations). We provide in Sect. 5 some guidance to help the user to implement these results. The probability distribution of the relative positions of associated sources is modeled in App. A.

2. Notations and general assumptions

We consider two catalogs K and K' defined on a common area S of the sky and use the following notations:

- $\#E$: number of elements of any set E ;
- M_1, \dots, M_n , with $n \equiv \#K$: sources in K ;

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¹ E.g., de Ruiter et al. (1977) state that, if there is a counterpart, the closest object is always the right one, which is obviously wrong.

- $M'_1, \dots, M'_{n'}$, with $n' \equiv \#K'$: sources in K' .

We define the following events:

- c_i : M_i is in the infinitesimal surface element $d^2\mathbf{r}_i$ located at \mathbf{r}_i ;
- c'_j : M'_j is in the surface element $d^2\mathbf{r}'_j$ located at \mathbf{r}'_j ;
- $C \equiv \bigcap_{i=1}^n c_i$: the coordinates of all K -sources are known;
- $C' \equiv \bigcap_{j=1}^{n'} c'_j$: the coordinates of all K' -sources are known;
- $A_{i,j}$, with $j > 0$: M'_j is the counterpart of M_i ;
- $A_{i,0}$: M_i has no counterpart in K' , i.e. $A_{i,0} = \overline{\bigcup_{j>0} A_{i,j}}$, where $\overline{\omega}$ denotes the negation of any event ω ;
- $A_{0,j}$: M'_j has no counterpart in K .

We also write f the *a priori* probability $P(\bigcup_{j>0} A_{i,j})$ that an element of K has a counterpart in K' (so, $P(A_{i,0}) = 1 - f$); we will see in Sects. 3.2 and 4.2 how to estimate f . We moreover assume that any M_i has at most one counterpart in K' : $A_{i,j} \cap A_{i,k} = \emptyset$ if $j \neq k$.

Clustering is neglected in all the paper.

3. Several-to-one associations

In this section, we do not make any assumption on the number of K -sources that may be the counterpart of a given source of K' : this is a reasonable hypothesis if the angular resolution in K' (e.g. IRAS) is much poorer than in K (e.g. LEDA), since, in that case, several distinct objects of K may be confused in K' . As evidenced by Sect. 3.3, this is also the assumption implicitly made by most of the authors cited in the introduction. We call this the “several-to-one” case.

3.1. Probability of association: all-sky computation

We want to compute², in the several-to-one case, the probability $P_{s:o}(A_{i,j} | C \cap C')$ of association of sources M_i and M'_j ($j > 0$) or the probability that M_i has no counterpart ($j = 0$), knowing the coordinates of all the objects in K and K' . Remembering that, for any events ω_1, ω_2 and ω_3 , $P(\omega_1 | \omega_2) = P(\omega_1 \cap \omega_2) / P(\omega_2)$ and $P(\omega_1 \cap \omega_2 | \omega_3) = P(\omega_1 | \omega_2 \cap \omega_3) P(\omega_2 | \omega_3)$, we have

$$P_{s:o}(A_{i,j} | C \cap C') = \frac{P_{s:o}(A_{i,j} \cap C \cap C')}{P_{s:o}(C \cap C')} = \frac{P_{s:o}(A_{i,j} \cap C | C')}{P_{s:o}(C | C')}. \quad (1)$$

We first compute $P_{s:o}(C | C')$. Using the symbol \uplus for mutually exclusive events instead of \cup , we obtain

$$\begin{aligned} P_{s:o}(C | C') &= P_{s:o}\left(C \cap \biguplus_{j_1=0}^{n'} \biguplus_{j_2=0}^{n'} \dots \biguplus_{j_n=0}^{n'} \bigcap_{k=1}^n A_{k,j_k} \mid C'\right) = \sum_{j_1=0}^{n'} \sum_{j_2=0}^{n'} \dots \sum_{j_n=0}^{n'} P_{s:o}\left(C \cap \bigcap_{k=1}^n A_{k,j_k} \mid C'\right) \\ &= \sum_{j_1=0}^{n'} \sum_{j_2=0}^{n'} \dots \sum_{j_n=0}^{n'} P_{s:o}\left(C \mid \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) P_{s:o}\left(\bigcap_{k=1}^n A_{k,j_k} \mid C'\right). \end{aligned} \quad (2)$$

One has

$$\begin{aligned} P_{s:o}\left(C \mid \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) &= P_{s:o}\left(c_1 \mid \bigcap_{k=2}^n c_k \cap \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) P_{s:o}\left(\bigcap_{k=2}^n c_k \mid \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) \\ &= \prod_{\ell=1}^n P_{s:o}\left(c_\ell \mid \bigcap_{k=\ell+1}^n c_k \cap \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) \end{aligned} \quad (3)$$

by iteration.

If $j_\ell \neq 0$, since M_ℓ is associated with M'_{j_ℓ} only,

$$P_{s:o}\left(c_\ell \mid \bigcap_{k=\ell+1}^n c_k \cap \bigcap_{k=1}^n A_{k,j_k} \cap C'\right) = P_{s:o}(c_\ell | A_{\ell,j_\ell} \cap c'_{j_\ell}) = \xi_{\ell,j_\ell} d^2\mathbf{r}_\ell, \quad (4)$$

where

$$\xi_{\ell,j_\ell} \equiv \frac{\exp\left(-\frac{1}{2} \mathbf{r}_{\ell,j_\ell}^\top \cdot \Gamma_{\ell,j_\ell}^{-1} \cdot \mathbf{r}_{\ell,j_\ell}\right)}{2\pi (\det \Gamma_{\ell,j_\ell})^{1/2}},$$

$\mathbf{r}_{\ell,j_\ell} \equiv \mathbf{r}'_{j_\ell} - \mathbf{r}_\ell$ and the covariance matrix Γ_{ℓ,j_ℓ} of \mathbf{r}_{ℓ,j_ℓ} is computed as detailed in App. A. (Note that, in the several-to-one case considered here, the computation of $P_{s:o}(C | C')$ is easier than that of $P_{s:o}(C' | C)$: because several M_ℓ may be associated with the

² For the sake of clarity, let us mention that we adopt the same decreasing order of precedence of operators as in *Mathematica* (Wolfram 1996): \times and $/$; $[]$; \sum ; $+$ and $-$.

same M'_k , the latter would require to calculate $P_{s:o}(c'_k | \bigcap_{\ell=1}^n [c_\ell \cap A_{\ell, j_\ell}])$. This does not matter in the one-to-one case studied in Sect. 4.)

If $j_\ell = 0$, since M_ℓ is not associated with any source in K' and clustering is neglected,

$$P_{s:o}(c_\ell | \bigcap_{k=\ell+1}^n c_k \cap \bigcap_{k=1}^{n'} c'_k \cap \bigcap_{k=1}^n A_{k, j_k}) = P_{s:o}(c_\ell | A_{\ell, 0}) = \xi_{\ell, 0} d^2 \mathbf{r}_\ell, \quad (5)$$

where $\xi_{\ell, 0} \equiv 1/S$ if we assume a uniform distribution of K -sources without counterpart as prior.

From Eqs. (3), (4) and (5), it follows that

$$P_{s:o}(C | \bigcap_{k=1}^n A_{k, j_k} \cap C') = \lambda \prod_{k=1}^n \xi_{k, j_k}, \quad (6)$$

where $\lambda \equiv \prod_{k=1}^n d^2 \mathbf{r}_k$.

We now compute $P_{s:o}(\bigcap_{k=1}^n A_{k, j_k} | C')$. Without any other assumption, $P_{s:o}(\bigcap_{k=1}^n A_{k, j_k} | C') = P_{s:o}(\bigcap_{k=1}^n A_{k, j_k})$. Let $m \equiv \#\{j_k > 0; k \in \llbracket 1, n \rrbracket\}$. Since a given M'_ℓ may be the counterpart of several M_k (i.e. the events $(A_{k, j_k})_{k \in \llbracket 1, n \rrbracket}$ are independent whatever the values of the indices j_k),

$$P_{s:o}(\bigcap_{k=1}^n A_{k, j_k}) = \prod_{k=1}^n P_{s:o}(A_{k, j_k}).$$

As $P_{s:o}(A_{k, 0}) = 1 - f$ and $P_{s:o}(A_{k, j_k}) = f/n'$ for $j_k > 0$,

$$P_{s:o}(\bigcap_{k=1}^n A_{k, j_k}) = \left(\frac{f}{n'}\right)^m (1 - f)^{n-m}. \quad (7)$$

Hence, from Eqs. (1), (2), (6) and (7),

$$P_{s:o}(C | C') = \lambda \sum_{j_1=0}^{n'} \sum_{j_2=0}^{n'} \cdots \sum_{j_n=0}^{n'} \left(\frac{f}{n'}\right)^m (1 - f)^{n-m} \prod_{k=1}^n \xi_{k, j_k} = \lambda L_{s:o}, \quad (8)$$

where

$$L_{s:o} \equiv \sum_{j_1=0}^{n'} \sum_{j_2=0}^{n'} \cdots \sum_{j_n=0}^{n'} \prod_{k=1}^n \xi_{k, j_k} = \prod_{k=1}^n \sum_{j_k=0}^{n'} \xi_{k, j_k} \quad (9)$$

is the likelihood to observe the K -sources at their positions if the positions of K' -sources are known, $\zeta_{k, 0} \equiv (1 - f) \xi_{k, 0}$ and $\zeta_{k, j_k} \equiv f \xi_{k, j_k} / n'$ if $j_k > 0$.

The computation of $P_{s:o}(A_{i, j} \cap C | C')$ is similar to that of $P_{s:o}(C | C')$:

$$\begin{aligned} P_{s:o}(A_{i, j} \cap C | C') &= P_{s:o}(C \cap A_{i, j} \cap \bigcup_{j_1=0}^{n'} \cdots \bigcup_{j_{i-1}=0}^{n'} \bigcup_{j_{i+1}=0}^{n'} \cdots \bigcup_{j_n=0}^{n'} \bigcap_{\substack{k=1 \\ k \neq i}}^n A_{k, j_k} | C') = P_{s:o}(C \cap \bigcup_{j_1=0}^{n'} \cdots \bigcup_{j_{i-1}=0}^{n'} \bigcup_{j_{i+1}=0}^{n'} \cdots \bigcup_{j_n=0}^{n'} \bigcap_{k=1}^n A_{k, j_k} | C') \\ &= \sum_{j_1=0}^{n'} \cdots \sum_{j_{i-1}=0}^{n'} \sum_{j_{i+1}=0}^{n'} \cdots \sum_{j_n=0}^{n'} P_{s:o}(C | \bigcap_{k=1}^n A_{k, j_k} \cap C') P_{s:o}(\bigcap_{k=1}^n A_{k, j_k} | C'), \end{aligned} \quad (10)$$

where we have put $j_i \equiv j$.

Let $m^* \equiv \#\{j_k > 0; k \in \llbracket 1, n \rrbracket\}$ (indices j_k are those of Eq. (10)). As for $P_{s:o}(C | C')$,

$$\begin{aligned} P_{s:o}(A_{i, j} \cap C | C') &= \lambda \sum_{j_1=0}^{n'} \cdots \sum_{j_{i-1}=0}^{n'} \sum_{j_{i+1}=0}^{n'} \cdots \sum_{j_n=0}^{n'} \left(\frac{f}{n'}\right)^{m^*} (1 - f)^{n-m^*} \prod_{k=1}^n \xi_{k, j_k} = \lambda \zeta_{i, j} \sum_{j_1=0}^{n'} \cdots \sum_{j_{i-1}=0}^{n'} \sum_{j_{i+1}=0}^{n'} \cdots \sum_{j_n=0}^{n'} \prod_{\substack{k=1 \\ k \neq i}}^n \xi_{k, j_k} \\ &= \lambda \zeta_{i, j} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \xi_{k, j_k}. \end{aligned} \quad (11)$$

Finally, from Eqs. (1), (8), (9) and (11),

$$P_{s:o}(A_{i, j} | C \cap C') = \frac{\zeta_{i, j} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \xi_{k, j_k}}{\prod_{k=1}^n \sum_{j_k=0}^{n'} \xi_{k, j_k}} = \frac{\zeta_{i, j}}{\sum_{k=0}^{n'} \xi_{i, k}} \quad (12)$$

$$= \begin{cases} \frac{f \xi_{i, j}}{(1 - f) n'/S + f \sum_{k=1}^{n'} \xi_{i, k}} & \text{if } j > 0, \\ \frac{(1 - f) n'/S}{(1 - f) n'/S + f \sum_{k=1}^{n'} \xi_{i, k}} & \text{if } j = 0. \end{cases} \quad (13)$$

The probability $P_{\text{s:o}}(A_{0,j} | C \cap C')$ that M_j' has no counterpart in K can be computed in this way:

$$\begin{aligned} P_{\text{s:o}}(A_{0,j} | C \cap C') &= P_{\text{s:o}}\left(C \cap A_{0,j} \cap \bigcup_{j_1=0}^{n'} \bigcup_{j_2=0}^{n'} \cdots \bigcup_{j_n=0}^{n'} \bigcap_{k=1}^n A_{k,j_k} \mid C'\right) = P_{\text{s:o}}\left(C \cap \bigcup_{\substack{j_1=0 \\ j_1 \neq j}}^{n'} \bigcup_{\substack{j_2=0 \\ j_2 \neq j}}^{n'} \cdots \bigcup_{\substack{j_n=0 \\ j_n \neq j}}^{n'} \bigcap_{k=1}^n A_{k,j_k} \mid C'\right) \\ &= \sum_{\substack{j_1=0 \\ j_1 \neq j}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \neq j}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \neq j}}^{n'} P_{\text{s:o}}\left(C \cap \bigcap_{k=1}^n A_{k,j_k} \mid C'\right) = \lambda \sum_{\substack{j_1=0 \\ j_1 \neq j}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \neq j}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \neq j}}^{n'} \prod_{k=1}^n \zeta_{k,j_k} = \lambda \prod_{k=1}^n \sum_{\substack{j_k=0 \\ j_k \neq j}}^{n'} \zeta_{k,j_k} \end{aligned}$$

and

$$\begin{aligned} P_{\text{s:o}}(A_{0,j} | C \cap C') &= \frac{P_{\text{s:o}}(A_{0,j} \cap C | C')}{P_{\text{s:o}}(C | C')} = \frac{\lambda \prod_{k=1}^n \sum_{\substack{j_k=0 \\ j_k \neq j}}^{n'} \zeta_{k,j_k}}{\lambda \prod_{k=1}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k}} = \prod_{k=1}^n \frac{\sum_{j_k=0}^{n'} \zeta_{k,j_k} - \zeta_{k,j}}{\sum_{j_k=0}^{n'} \zeta_{k,j_k}} = \prod_{k=1}^n \left(1 - \frac{\zeta_{k,j}}{\sum_{j_k=0}^{n'} \zeta_{k,j_k}}\right) \\ &= \prod_{k=1}^n (1 - P_{\text{s:o}}[A_{k,j} | C \cap C']). \end{aligned} \quad (14)$$

3.2. Fraction of sources with a counterpart and other unknown parameters

3.2.1. Estimates

Besides f , the probabilities $P(A_{i,j} | C \cap C')$ may depend on other unknown parameters, e.g. $\hat{\sigma}$ and $\hat{\nu}$ (cf. App. A). Let us write them x_1, x_2 , etc., and $\mathbf{x} \equiv (x_1, x_2, \dots)$. An estimate $\hat{\mathbf{x}}$ of \mathbf{x} may be obtained by maximizing the likelihood L with respect to \mathbf{x} (and with the constraint $\hat{f}_{\text{s:o}} \in [0, 1]$), or, equivalently, by finding the solution $\hat{\mathbf{x}}$ of

$$\frac{\partial \ln L}{\partial \mathbf{x}} = 0. \quad (15)$$

For any parameter x_p , as all the $\zeta_{i,j}$ are strictly positive and $\ln L_{\text{s:o}} = \sum_{i=1}^n \ln \sum_{k=0}^{n'} \zeta_{i,k}$ (Eq. (9)),

$$\begin{aligned} \frac{\partial \ln L_{\text{s:o}}}{\partial x_p} &= \sum_{i=1}^n \frac{\partial \ln \sum_{k=0}^{n'} \zeta_{i,k}}{\partial x_p} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \zeta_{i,j} / \partial x_p}{\sum_{k=0}^{n'} \zeta_{i,k}} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \frac{\zeta_{i,j}}{\sum_{k=0}^{n'} \zeta_{i,k}} \\ &= \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} P_{\text{s:o}}(A_{i,j} | C \cap C'). \end{aligned} \quad (16)$$

Let us consider in particular the case $x_p = f$. Note that $\partial \ln \zeta_{i,0} / \partial f = -1/(1-f)$ and $\partial \ln \zeta_{i,j} / \partial f = 1/f$ for $j > 0$. Since $\sum_{j=0}^{n'} P_{\text{s:o}}(A_{i,j} | C \cap C') = 1$,

$$\begin{aligned} \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} P_{\text{s:o}}(A_{i,j} | C \cap C') &= -\frac{P_{\text{s:o}}(A_{i,0} | C \cap C')}{1-f} + \sum_{j=1}^{n'} \frac{P_{\text{s:o}}(A_{i,j} | C \cap C')}{f} = -\frac{P_{\text{s:o}}(A_{i,0} | C \cap C')}{1-f} + \frac{1 - P_{\text{s:o}}(A_{i,0} | C \cap C')}{f} \\ &= \frac{(1-f) - P_{\text{s:o}}(A_{i,0} | C \cap C')}{f(1-f)}. \end{aligned} \quad (17)$$

Summing on i , we obtain

$$\frac{\partial \ln L_{\text{s:o}}}{\partial f} = \frac{n(1-f) - \sum_{i=1}^n P_{\text{s:o}}(A_{i,0} | C \cap C')}{f(1-f)}. \quad (18)$$

So, as expected, an estimate of the probability that a source in K has a counterpart in K' is given by

$$\hat{f}_{\text{s:o}} = 1 - \frac{1}{n} \sum_{i=1}^n \hat{P}_{\text{s:o}}(A_{i,0} | C \cap C'), \quad (19)$$

$$= \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{n'} \hat{P}_{\text{s:o}}(A_{i,j} | C \cap C'). \quad (20)$$

Note that, since $\partial^2 \zeta_{i,j} / \partial f^2 = 0$ for all $(i, j) \in \llbracket 1, n \rrbracket \times \llbracket 0, n' \rrbracket$,

$$\frac{\partial^2 \ln L_{\text{s:o}}}{\partial f^2} = - \sum_{i=1}^n \left(\frac{\sum_{j=0}^{n'} \partial \zeta_{i,j} / \partial f}{\sum_{j=0}^{n'} \zeta_{i,j}} \right)^2 < 0 \quad (21)$$

for all f , so $\partial \ln L_{s:o} / \partial f$ has at most one zero in $[0, 1]$: $\hat{f}_{s:o}$ is unique.

One may also compute an estimate of the fraction f' of K' -sources with a counterpart from

$$\hat{f}'_{s:o} = 1 - \frac{1}{n'} \sum_{j=1}^{n'} \hat{P}_{s:o}(A_{0,j} | C \cap C'). \quad (22)$$

One can easily check from Eqs. (20), (22) and (14) that $\hat{f}_{s:o}/n' > \hat{f}'_{s:o}/n$ in the several-to-one case.

3.2.2. Uncertainties

It may be interesting to know the uncertainties on the unknown parameters. For large numbers of sources, the covariance matrix V of $\hat{\mathbf{x}}$ is asymptotically given by

$$(V^{-1})_{p,q} = \left(-\frac{\partial^2 \ln L}{\partial x_p \partial x_q} \right)_{\mathbf{x}=\hat{\mathbf{x}}} \quad (23)$$

(Kendall & Stuart 1979).

Let us write with a circumflex accent all the quantities calculated at $\mathbf{x} = \hat{\mathbf{x}}$. From

$$\frac{\partial^2 \ln L}{\partial x_p \partial x_q} = \frac{1}{P(C | C')} \frac{\partial^2 P(C | C')}{\partial x_p \partial x_q} - \frac{1}{P^2(C | C')} \frac{\partial P(C | C')}{\partial x_p} \frac{\partial P(C | C')}{\partial x_q},$$

one obtains

$$\frac{\hat{\partial}^2 \ln L}{\hat{\partial} x_p \hat{\partial} x_q} = \frac{1}{\hat{P}(C | C')} \frac{\hat{\partial}^2 P(C | C')}{\hat{\partial} x_p \hat{\partial} x_q}. \quad (24)$$

One has

$$\frac{\partial^2 P_{s:o}(C | C')}{\partial x_p \partial x_q} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial^2 \ln \zeta_{i,j}}{\partial x_p \partial x_q} P_{s:o}(A_{i,j} \cap C | C') + \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \frac{\partial P_{s:o}(A_{i,j} \cap C | C')}{\partial x_q}. \quad (25)$$

For any product of strictly positive functions g_k of some variable y ,

$$\frac{\partial \prod_{k=1}^n g_k}{\partial y} = \sum_{i=1}^n \frac{\partial g_i}{\partial y} \prod_{\substack{k=1 \\ k \neq i}}^n g_k = \sum_{i=1}^n \frac{\partial \ln g_i}{\partial y} \prod_{k=1}^n g_k, \quad (26)$$

so, using Eq. (11),

$$\begin{aligned} \frac{\partial P_{s:o}(A_{i,j} \cap C | C')}{\partial x_q} &= \lambda \frac{\partial \zeta_{i,j}}{\partial x_q} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} + \lambda \zeta_{i,j} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \frac{\partial \sum_{j_\ell=0}^{n'} \zeta_{\ell,j_\ell}}{\partial x_q} \prod_{\substack{k=1 \\ k \notin \{i,\ell\}}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} \\ &= \lambda \frac{\partial \ln \zeta_{i,j}}{\partial x_q} \zeta_{i,j} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} + \lambda \frac{\zeta_{i,j}}{\sum_{j_i=0}^{n'} \zeta_{i,j_i}} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell,j_\ell}}{\partial x_q} \zeta_{\ell,j_\ell} \prod_{\substack{k=1 \\ k \neq \ell}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} \\ &= \frac{\partial \ln \zeta_{i,j}}{\partial x_q} P_{s:o}(A_{i,j} \cap C | C') + P_{s:o}(A_{i,j} | C \cap C') \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell,j_\ell}}{\partial x_q} P_{s:o}(A_{\ell,j_\ell} \cap C | C'). \end{aligned} \quad (27)$$

For $\mathbf{x} = \hat{\mathbf{x}}$,

$$\begin{aligned} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\hat{\partial} \ln \zeta_{\ell,j_\ell}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{\ell,j_\ell} \cap C | C') &= \sum_{\ell=1}^n \sum_{j_\ell=0}^{n'} \frac{\hat{\partial} \ln \zeta_{\ell,j_\ell}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{\ell,j_\ell} \cap C | C') - \sum_{j_i=0}^{n'} \frac{\hat{\partial} \ln \zeta_{i,j_i}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{i,j_i} \cap C | C') \\ &= - \sum_{j_i=0}^{n'} \frac{\hat{\partial} \ln \zeta_{i,j_i}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{i,j_i} \cap C | C') \end{aligned} \quad (28)$$

since the first term on the right-hand side of the first line is zero from Eq. (16). Finally, combining Eqs. (25), (27), (28) and dividing by $\hat{P}_{s:o}(C | C')$, we obtain

$$\begin{aligned} \frac{\partial^2 \ln L_{s:o}}{\partial x_p \partial x_q} &= \sum_{i=1}^n \sum_{j=0}^{n'} \left(\frac{\partial^2 \ln \zeta_{i,j}}{\partial x_p \partial x_q} + \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \frac{\partial \ln \zeta_{i,j}}{\partial x_q} \right) \hat{P}_{s:o}(A_{i,j} | C \cap C') \\ &\quad - \sum_{i=1}^n \left(\sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \hat{P}_{s:o}[A_{i,j} | C \cap C'] \right) \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_q} \hat{P}_{s:o}(A_{i,j} | C \cap C'). \end{aligned} \quad (29)$$

In particular, for $x_p = x_q = f$, $\partial^2 \ln \zeta_{i,j} / \partial f^2 + (\partial \ln \zeta_{i,j} / \partial f)^2 = 0$, whether $j = 0$ or not. From Eqs. (17) and (19),

$$\begin{aligned} \frac{\partial^2 \ln L_{s:o}}{\partial f^2} &= - \sum_{i=1}^n \left(\frac{1}{\hat{f}_{s:o}} - \frac{\hat{P}_{s:o}[A_{i,0} | C \cap C']}{\hat{f}_{s:o} (1 - \hat{f}_{s:o})} \right)^2 \\ &= \frac{n}{\hat{f}_{s:o}^2} - \frac{\sum_{i=1}^n \hat{P}_{s:o}^2(A_{i,0} | C \cap C')}{\hat{f}_{s:o}^2 (1 - \hat{f}_{s:o})^2}. \end{aligned} \quad (30)$$

3.3. Probability of association: local computation

In the several-to-one case, a purely local computation of the probability of association between a given M_i and some M'_j ($j > 0$), or of the probability that M_i has no counterpart in K' , is also possible.

Let us consider a region D_i of area S_i containing the position of M_i , and such that we can safely hypothesize that the K' -counterpart of M_i , if any, will be inside. We assume that the local surface density ρ'_i of K' -sources unrelated to M_i is uniform on D_i . To avoid biasing the estimate if M_i has a counterpart, ρ'_i may be computed from the number of K' -sources in a region surrounding, but not overlapping, D_i .

Besides the $A_{i,j}$, we consider the following events:

- N'_i : D_i contains n'_i sources;
- $C'_i \equiv \bigcap_{j \in I_i} C'_j$, where $I_i \equiv \{j \mid M'_j \in D_i\}$.

We want to compute the probability that a source M'_j in D_i is the counterpart of M_i , given the positions of the neighbors, i.e. $P_{\text{loc}}(A_{i,j} | C'_i \cap N'_i)$. We have

$$\begin{aligned} P_{\text{loc}}(A_{i,j} | C'_i \cap N'_i) &= \frac{P_{\text{loc}}(A_{i,j} \cap C'_i \cap N'_i)}{P_{\text{loc}}(C'_i \cap N'_i)} = \frac{P_{\text{loc}}(C'_i \cap A_{i,j} \cap N'_i)}{P_{\text{loc}}(C'_i \cap \bigcup_{k \in I_i \cup \{0\}} A_{i,k} \cap N'_i)} \\ &= \frac{P_{\text{loc}}(C'_i \cap A_{i,j} \cap N'_i)}{\sum_{k \in I_i \cup \{0\}} P_{\text{loc}}(C'_i \cap A_{i,k} \cap N'_i)} = \frac{P_{\text{loc}}(C'_i | A_{i,j} \cap N'_i) P_{\text{loc}}(A_{i,j} \cap N'_i)}{\sum_{k \in I_i \cup \{0\}} P_{\text{loc}}(C'_i | A_{i,k} \cap N'_i) P_{\text{loc}}(A_{i,k} \cap N'_i)} \\ &= \frac{P_{\text{loc}}(C'_i | A_{i,j} \cap N'_i) P_{\text{loc}}(A_{i,j} | N'_i)}{\sum_{k \in I_i \cup \{0\}} P_{\text{loc}}(C'_i | A_{i,k} \cap N'_i) P_{\text{loc}}(A_{i,k} | N'_i)}. \end{aligned}$$

If $j > 0$, $P_{\text{loc}}(A_{i,j} | N'_i) = P_{\text{loc}}(\bigcup_{k \in I_i} A_{i,k} | N'_i) / n'_i$ (one sees here why the event N'_i was defined: otherwise, $P_{\text{loc}}(A_{i,j})$ could not be computed as $P_{\text{loc}}(\bigcup_{k \in I_i} A_{i,k}) / n'_i$ because n'_i would be undefined). Now,

$$P_{\text{loc}}\left(\bigcup_{k \in I_i} A_{i,k} | N'_i\right) = \frac{P_{\text{loc}}(N'_i \cap \bigcup_{k \in I_i} A_{i,k})}{P_{\text{loc}}(N'_i)} = \frac{P_{\text{loc}}(N'_i | \bigcup_{k \in I_i} A_{i,k}) P_{\text{loc}}(\bigcup_{k \in I_i} A_{i,k})}{P_{\text{loc}}(N'_i | A_{i,0}) P_{\text{loc}}(A_{i,0}) + P_{\text{loc}}(N'_i | \bigcup_{k \in I_i} A_{i,k}) P_{\text{loc}}(\bigcup_{k \in I_i} A_{i,k})}.$$

If clustering is negligible, the number of sources randomly distributed with a mean surface density ρ'_i in an area S_i follows a Poissonian distribution, so

$$P_{\text{loc}}(N'_i | \bigcup_{k \in I_i} A_{i,k}) = \frac{(\rho'_i S_i)^{n'_i-1} \exp(-\rho'_i S_i)}{(n'_i - 1)!} \quad (n'_i - 1 \text{ random sources in } S_i)$$

and

$$P_{\text{loc}}(N'_i | A_{i,0}) = \frac{(\rho'_i S_i)^{n'_i} \exp(-\rho'_i S_i)}{n'_i!} \quad (n'_i \text{ random sources in } S_i).$$

Thus,

$$P_{\text{loc}}(A_{i,j} | N'_i) = \begin{cases} \frac{f}{n'_i f + (1-f) \rho'_i S_i} & \text{if } j > 0, \\ \frac{(1-f) \rho'_i S_i}{n'_i f + (1-f) \rho'_i S_i} & \text{if } j = 0. \end{cases}$$

For $j > 0$,

$$P_{\text{loc}}(C'_i | A_{i,j} \cap N'_i) = \xi_{i,j} d^2 r'_j \prod_{\substack{k \in I_i \\ k \neq j}} \frac{d^2 r'_k}{S_i}$$

(rigorously, $\xi_{i,j}$ should be replaced by $\xi_{i,j}/P_{\text{loc}}(M'_j \in D_i | A_{i,j})$, but $P_{\text{loc}}(M'_j \notin D_i | A_{i,j})$ is negligible), and

$$P_{\text{loc}}(C'_i | A_{i,0} \cap N'_i) = \prod_{k \in I_i} \frac{d^2 r'_k}{S_i}.$$

Finally,

$$P_{\text{loc}}(A_{i,j} | C'_i \cap N'_i) = \begin{cases} \frac{f \text{LR}_{i,j}}{(1-f) + f \sum_{k \in I_i} \text{LR}_{i,k}} & \text{if } j > 0, \\ \frac{(1-f)}{(1-f) + f \sum_{k \in I_i} \text{LR}_{i,k}} & \text{if } j = 0, \end{cases} \quad (31)$$

where $\text{LR}_{i,k} \equiv \xi_{i,k}/\rho'_i$ is the “likelihood ratio”. *Mutatis mutandis*, one obtains the same result as Eq. (14) of Pineau et al. (2011) and aforementioned authors. When extended to the all sky (i.e. $S_i \rightarrow S$), ρ'_i is replaced by n'/S in Eq. (31), $\sum_{k \in I_i}$ by $\sum_{k=1}^{n'}$ and one recovers Eq. (13).

The index \check{j}_i of the most likely counterpart $M'_{\check{j}_i}$ of M_i is the value of $j > 0$ maximizing $\text{LR}_{i,j}$. Usually, $\sum_{k=1; k \neq \check{j}_i}^{n'} \text{LR}_{i,k} \ll \text{LR}_{i,\check{j}_i}$, so

$$P_{\text{s.o.}}(A_{i,\check{j}_i} | C \cap C') \approx \frac{f \text{LR}_{i,\check{j}_i}}{(1-f) + f \text{LR}_{i,\check{j}_i}}.$$

As a “poor man’s” recipe, if the value of f is unknown and not too close to either 0 or 1, an association may be considered as true if $\text{LR}_{i,\check{j}_i} \gg 1$ and as false if $\text{LR}_{i,\check{j}_i} \ll 1$. Where to set the boundary between true associations and false ones is somewhat arbitrary. For a large sample, however, f can be determined from the distribution of the positions of all the sources, as shown in Sect. 3.2.

4. One-to-one associations

In Sect. 3, a given M'_j may be associated with several M_i : the probabilities are actually asymmetric in M_i and M'_j and, while $\sum_{j=0}^{n'} P_{\text{s.o.}}(A_{i,j} | C \cap C') = 1$ for all M_i , one may well have $\sum_{i=1}^n P_{\text{s.o.}}(A_{i,j} | C \cap C') > 1$ for some sources M'_j .

Here, we assume not only that each K -source is associated with at most one K' -source, but that each K' -source is associated with at most one K -source. We call this the “one-to-one” case and note $P_{\text{o.o.}}$ the probabilities calculated under this assumption. As far as we know and despite some attempt by Rutledge et al. (2000), this problem has not been solved previously.

Since a K' -potential counterpart of M_i within some neighborhood D_i of M_i might in fact be the true counterpart of another source M_k outside of D_i , there is no obvious way to extend the exact local several-to-one computation of Sect. 3.3 to the one-to-one case. We therefore have to consider either the whole sky, as in Sect. 3.1, or at least some large enough region around both M_i and M'_j to neglect side effects.

In the case of one-to-one associations, a source of K and a source of K' play symmetrical roles; in particular, $P_{\text{o.o.}}(A_{i,j}) = f/n' = f'/n$. However, for practical reasons (cf. Eq. (36)), we name K the catalog with the fewer objects and K' the other one, so $n \leq n'$ in the following.

4.1. Probability of association

We want to compute $P_{\text{o.o.}}(A_{i,j} | C \cap C')$ for $i > 0$. We still have

$$P_{\text{o.o.}}(A_{i,j} | C \cap C') = \frac{P_{\text{o.o.}}(A_{i,j} \cap C | C')}{P_{\text{o.o.}}(C | C')} \quad (32)$$

and

$$P_{\text{o.o.}}(C | C') = P_{\text{o.o.}}\left(C \cap \bigcup_{j_1=0}^{n'} \bigcup_{j_2=0}^{n'} \cdots \bigcup_{j_n=0}^{n'} \bigcap_{k=1}^n A_{k,j_k} \mid C'\right).$$

As $A_{i,j} \cap A_{k,\ell} = \emptyset$ if $i \neq k$ and $j = \ell > 0$, this reduces to

$$P_{\text{o.o.}}(C | C') = P_{\text{o.o.}}\left(C \cap \bigcup_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \bigcup_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \bigcup_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \bigcap_{k=1}^n A_{k,j_k} \mid C'\right),$$

where $J_0 \equiv \emptyset$ and J_k is defined iteratively for all $k \in \llbracket 1, n \rrbracket$ by $J_k \equiv (J_{k-1} \cup \{j_k\}) \setminus \{0\}$. Hence,

$$\begin{aligned} P_{\text{o:o}}(C \mid C') &= \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} P_{\text{o:o}}\left(C \cap \bigcap_{k=1}^n A_{k, j_k} \mid C'\right) \\ &= \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} P_{\text{o:o}}\left(C \mid \bigcap_{k=1}^n A_{k, j_k} \cap C'\right) P_{\text{o:o}}\left(\bigcap_{k=1}^n A_{k, j_k} \mid C'\right). \end{aligned} \quad (33)$$

As in the several-to-one case,

$$P_{\text{o:o}}\left(C \mid \bigcap_{k=1}^n A_{k, j_k} \cap C'\right) = \lambda \prod_{k=1}^n \xi_{k, j_k}. \quad (34)$$

We now have to compute $P_{\text{o:o}}(\bigcap_{k=1}^n A_{k, j_k} \mid C') = P_{\text{o:o}}(\bigcap_{k=1}^n A_{k, j_k})$. Let $m \equiv \#J_n$ and X be a random variable describing the number of associations between K and K' :

$$P_{\text{o:o}}\left(\bigcap_{k=1}^n A_{k, j_k}\right) = P_{\text{o:o}}\left(\bigcap_{k=1}^n A_{k, j_k} \mid X = m\right) P_{\text{o:o}}(X = m) + P_{\text{o:o}}\left(\bigcap_{k=1}^n A_{k, j_k} \mid X \neq m\right) P_{\text{o:o}}(X \neq m).$$

Since $P_{\text{o:o}}(\bigcap_{k=1}^n A_{k, j_k} \mid X \neq m) = 0$, one just has to compute $P_{\text{o:o}}(\bigcap_{k=1}^n A_{k, j_k} \mid X = m)$ and $P_{\text{o:o}}(X = m)$.

There are $n!/(m! [n - m]!)$ choices of m elements among n in K , and $n'!/(m! [n' - m]!)$ of m elements among n' in K' . The number of permutations of m elements is $m!$, so the total number of one-to-one associations of m elements from K to m elements of K' is

$$m! \frac{n!}{m! (n - m)!} \frac{n'!}{m! (n' - m)!}.$$

The inverse of this number is

$$P_{\text{o:o}}\left(\bigcap_{k=1}^n A_{k, j_k} \mid X = m\right) = \frac{m! (n - m)! (n' - m)!}{n! n'!}. \quad (35)$$

With our definition of K and K' , $n \leq n'$, so all the elements of K may have a counterpart in K' jointly. Therefore, $P_{\text{o:o}}(X = m)$ is given by the binomial law:

$$P_{\text{o:o}}(X = m) = \frac{n!}{m! (n - m)!} f^m (1 - f)^{n - m}. \quad (36)$$

From Eqs. (33), (34), (35) and (36), we obtain

$$\begin{aligned} P_{\text{o:o}}(C \mid C') &= \lambda \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \frac{(n' - m)!}{n'!} f^m (1 - f)^{n - m} \prod_{k=1}^n \xi_{k, j_k} \\ &= \lambda L_{\text{o:o}}, \end{aligned} \quad (37)$$

where

$$L_{\text{o:o}} \equiv \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \prod_{k=1}^n \eta_{k, j_k}, \quad (38)$$

$\eta_{k, 0} \equiv \zeta_{k, 0}$ and $\eta_{k, j_k} \equiv f \xi_{k, j_k} / (n' - \#J_{k-1})$ if $j_k > 0$.

$P_{\text{o:o}}(A_{i, j} \cap C \mid C')$ is computed in the same way as $P_{\text{o:o}}(C \mid C')$:

$$\begin{aligned} P_{\text{o:o}}(A_{i, j} \cap C \mid C') &= P_{\text{o:o}}\left(C \cap A_{i, j} \cap \bigcup_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \bigcup_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \bigcup_{\substack{j_{i+1}=0 \\ j_{i+1} \notin J_i^*}}^{n'} \cdots \bigcup_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} \bigcap_{\substack{k=1 \\ k \neq i}}^n A_{k, j_k} \mid C'\right) \\ &= P_{\text{o:o}}\left(C \cap \bigcup_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \bigcup_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \bigcup_{\substack{j_{i+1}=0 \\ j_{i+1} \notin J_i^*}}^{n'} \cdots \bigcup_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} \bigcap_{k=1}^n A_{k, j_k} \mid C'\right), \end{aligned}$$

where $j_i \equiv j$, $J_0^* \equiv \{j\} \setminus \{0\}$ and $J_k^* \equiv (J_{k-1}^* \cup \{j_k\}) \setminus \{0\}$ for all $k \in \llbracket 1, n \rrbracket$, so

$$P_{0:0}(A_{i,j} \cap C \mid C') = \sum_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \sum_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \sum_{\substack{j_i=0 \\ j_i \notin J_i^*}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} P_{0:0}(C \mid \bigcap_{k=1}^n A_{k,j_k} \cap C') P_{0:0}(\bigcap_{k=1}^n A_{k,j_k} \mid C').$$

Let $m^* \equiv \#J_n^*$. As for $P_{0:0}(C \mid C')$,

$$\begin{aligned} P_{0:0}(A_{i,j} \cap C \mid C') &= \lambda \sum_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \sum_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \sum_{\substack{j_i=0 \\ j_i \notin J_i^*}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} \frac{(n' - m^*)!}{n'!} f^{m^*} (1 - f)^{n - m^*} \prod_{k=1}^n \xi_{k,j_k} \\ &= \lambda \eta_{i,j}^* \sum_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \sum_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \sum_{\substack{j_i=0 \\ j_i \notin J_i^*}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} \prod_{\substack{k=1 \\ k \neq i}}^n \eta_{k,j_k}^*, \end{aligned} \quad (39)$$

where $\eta_{k,j_k}^* \equiv f \xi_{k,j_k} / (n' - \#J_{k-1}^*)$ if $k \neq i$ and $j_k > 0$, and $\eta_{k,j_k}^* = \zeta_{k,j_k}$ otherwise.

Finally, from Eqs. (32), (37), (38) and (39),

$$P_{0:0}(A_{i,j} \mid C \cap C') = \frac{\zeta_{i,j} \sum_{\substack{j_1=0 \\ j_1 \notin J_0^*}}^{n'} \cdots \sum_{\substack{j_{i-1}=0 \\ j_{i-1} \notin J_{i-2}^*}}^{n'} \sum_{\substack{j_i=0 \\ j_i \notin J_i^*}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}^*}}^{n'} \prod_{\substack{k=1 \\ k \neq i}}^n \eta_{k,j_k}^*}{\sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \prod_{k=1}^n \eta_{k,j_k}}. \quad (40)$$

The probability that a source M'_j has no counterpart in K is simply given by

$$P_{0:0}(A_{0,j} \mid C \cap C') = 1 - \sum_{k=1}^n P_{0:0}(A_{k,j} \mid C \cap C').$$

4.2. Fraction of sources with a counterpart and other unknown parameters

4.2.1. Estimates

As in the several-to-one case, an estimate $\hat{\mathbf{x}}_{0:0}$ of the set \mathbf{x} of unknown parameters may be obtained by solving Eq. (15) (with the constraint $\hat{f}_{0:0} \in [0, n/n']$). As the number of terms in $L_{0:0}$ grows exponentially with n and n' , Eq. (38) seems useless for this purpose. Fortunately, the computation of $L_{0:0}$ is not necessary if the probabilities $P_{0:0}(A_{i,j} \mid C \cap C')$ are known (we will see in Sect. 5.2 how to approximate these).

Indeed, for any parameter x_p , let us show that we get the same result (Eq. (16)) as in the several-to-one case. Using Eq. (26), we obtain

$$\frac{\partial P_{0:0}(C \mid C')}{\partial x_p} = \lambda \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \sum_{i=1}^n \frac{\partial \ln \eta_{i,j_i}}{\partial x_p} \prod_{k=1}^n \eta_{k,j_k}. \quad (41)$$

The expression of $P_{0:0}(A_{i,j} \cap C \mid C')$ may also be written

$$P_{0:0}(A_{i,j} \cap C \mid C') = \lambda \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \mathbf{1}(j_i = j) \prod_{k=1}^n \eta_{k,j_k},$$

where $\mathbf{1}$ is the indicator function (i.e. $\mathbf{1}(j_i = j) = 1$ if proposition “ $j_i = j$ ” is true and $\mathbf{1}(j_i = j) = 0$ otherwise), so

$$\begin{aligned} \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} P_{0:0}(A_{i,j} \cap C \mid C') &= \lambda \sum_{i=1}^n \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \sum_{j=0}^{n'} \mathbf{1}(j_i = j) \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \prod_{k=1}^n \eta_{k,j_k} \\ &= \lambda \sum_{i=1}^n \sum_{\substack{j_1=0 \\ j_1 \notin J_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin J_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin J_{n-1}}}^{n'} \frac{\partial \ln \zeta_{i,j_i}}{\partial x_p} \prod_{k=1}^n \eta_{k,j_k}. \end{aligned} \quad (42)$$

If $j_i = 0$, $\eta_{i,j_i} = \zeta_{i,j_i}$; and if $j_i > 0$, the numerators of η_{i,j_i} and ζ_{i,j_i} are the same and their denominators do not depend on x_p : in all cases, $\partial \ln \eta_{i,j_i} / \partial x_p = \partial \ln \zeta_{i,j_i} / \partial x_p$. The right-hand sides of Eqs. (41) and (42) are therefore identical. Dividing their left-hand sides by $P_{0:0}(C \mid C')$, one obtains again

$$\frac{\partial \ln L_{0:0}}{\partial x_p} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} P_{0:0}(A_{i,j} \mid C \cap C'). \quad (43)$$

For $x_p = f$, one still has $\partial \ln \zeta_{i,0} / \partial f = -1/(1-f)$ and $\partial \ln \zeta_{i,j} / \partial f = 1/f$ if $j > 0$, so, as in the several-to-one case,

$$\frac{\partial \ln L_{o:o}}{\partial f} = \frac{n(1-f) - \sum_{i=1}^n P_{o:o}(A_{i,0} | C \cap C')}{f(1-f)}. \quad (44)$$

4.2.2. Uncertainties

Regarding uncertainties on the x_p , Eqs. (23), (24) and (25) are valid in the one-to-one case too, so, from Eq. (43),

$$\frac{\partial^2 \ln L_{o:o}}{\partial x_p \partial x_q} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial^2 \ln \zeta_{i,j}}{\partial x_p \partial x_q} \hat{P}_{o:o}(A_{i,j} | C \cap C') + \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \frac{\partial P_{o:o}(A_{i,j} | C \cap C')}{\partial x_q}.$$

Contrary to the several-to-one case, no simple exact analytic expression of the terms $\partial P_{o:o}(A_{i,j} | C \cap C') / \partial x_q$ could be obtained. These derivatives may be computed numerically using finite differences; however, unless the fraction of sources having several likely counterparts is high, Eqs. (29) and (30) should provide a more convenient approximation of the covariance matrix of $\hat{\mathbf{x}}_{o:o}$.

5. Practical implementation

5.1. Several-to-one case

5.1.1. Neighbors only!

In the several-to-one case, the computation of the probability of association $P_{s:o}(A_{i,j} | C \cap C')$ between M_i and M'_j from Eq. (12) is without problem if f and the positional uncertainties are known. However, the number of calculations for the whole sample or for the determination of $\hat{\mathbf{x}}$ is of the order of $n n'^2$.

As $\zeta_{i,k}$ rapidly tends to 0 when the angular distance $r_{i,k}$ between M_i and M'_k increases, there is no need to sum from $k = 1$ to n' in Eq. (12), nor to compute explicitly all the $P_{s:o}(A_{i,j} | C \cap C')$. If R is some angular distance above which $\zeta_{i,k} \ll n'/S$, one may set $\zeta_{i,k}$ to 0 (and $P_{s:o}(A_{i,k})$ too) if $r_{i,k} > R$ and replace the sums $\sum_{k=1}^{n'}$ by $\sum_{k=1; r_{i,k} \leq R}^{n'}$.

In fact, for most M_i , one does not even need to test whether $r_{i,k} \leq R$ for each $M'_k \in K'$. Let us write E_i the domain of right ascensions α' out of which no point M' of declination δ' closer than R to M_i may be found. The angular distance ψ between M' and M_i is given (cf. Eq. (A.1)) by

$$\cos \psi = \cos(\alpha' - \alpha_i) \cos \delta_i \cos \delta' + \sin \delta_i \sin \delta'.$$

If $\delta_i \in [-\pi/2 + R, \pi/2 - R]$, the minimum of $\cos(\alpha' - \alpha_i)$ under the constraint $\cos \psi \geq \cos R$ is reached when $\sin \delta' = \sin \delta_i / \cos R$ and

$$\cos(\alpha' - \alpha_i) = \frac{\sqrt{\cos^2 R - \sin^2 \delta_i}}{\cos \delta_i}.$$

Let $\Delta_i \equiv \arccos(\sqrt{\cos^2 R - \sin^2 \delta_i} / \cos \delta_i)$. The domain E_i is given by

$$E_i = \begin{cases} [0, \alpha_i + \Delta_i - 2\pi] \cup [\alpha_i - \Delta_i, 2\pi] & \text{if } \alpha_i + \Delta_i > 2\pi, \\ [0, \alpha_i + \Delta_i] \cup [\alpha_i - \Delta_i + 2\pi, 2\pi] & \text{if } \alpha_i - \Delta_i < 0, \\ [\alpha_i - \Delta_i, \alpha_i + \Delta_i] & \text{otherwise.} \end{cases}$$

If $\delta_i \in [-\pi/2, -\pi/2 + R] \cup [\pi/2 - R, \pi/2]$, one has $E_i = [0, 2\pi]$.

For a catalog K' ordered by increasing right ascension (if not, this is the first thing to do), one may easily find the subset of indices k for which $\alpha'_k \in E_i$. For instance, if $E_i = [\alpha_i - \Delta_i, \alpha_i + \Delta_i]$, one just has to find by dichotomy the indices k^- and k^+ such that $\alpha'_{k^- - 1} < \alpha_i - \Delta_i \leq \alpha'_{k^-}$ and $\alpha'_{k^+} \leq \alpha_i + \Delta_i < \alpha'_{k^+ + 1}$. The sums $\sum_{k=1; r_{i,k} \leq R}^{n'}$ may then be replaced by $\sum_{k=k^-; r_{i,k} \leq R}^{k^+}$.

In all cases, the sum may be further restricted to sources with a declination $\delta'_k \in [\delta_i - R, \delta_i + R] \cap [-\pi/2, \pi/2]$.

5.1.2. Fraction of sources with a counterpart

All the probabilities depend on f and, possibly, other unknown parameters like $\hat{\sigma}$ and \hat{v} . These parameters may be found by solving Eq. (15) using Eq. (16).

If the fraction of sources with a counterpart is the only unknown, the $\xi_{i,j}$ need to be computed only once and f may be easily determined from Eq. (19). Denote g the function

$$g: [0, 1] \rightarrow \mathbb{R},$$

$$f \mapsto 1 - \frac{1}{n} \sum_{i=1}^n P_{s:o}(A_{i,0} | C \cap C').$$

Let us show that, for any $f_0 \in]0, 1[$, the sequence $(f_k)_{k \in \mathbb{N}}$ defined by $f_{k+1} \equiv g(f_k)$ tends to \hat{f} .

First, note that

$$g(f) = f + \frac{f(1-f)}{n} \frac{\partial \ln L_{s:o}}{\partial f}.$$

The only fixed points of g are hence 0, 1 and \hat{f} . As $\partial^2 \ln L_{s:o} / \partial f^2 < 0$ (Eq. (21)), one has $\partial \ln L_{s:o} / \partial f \geq 0$ and thus $g(f) \geq f$ for $f \in [0, \hat{f}]$; similarly, $\partial \ln L_{s:o} / \partial f \leq 0$ and $g(f) \leq f$ for $f \in [\hat{f}, 1]$. Because

$$\frac{dg}{df} = \frac{1}{n n'} \sum_{i=1}^n \frac{\xi_{i,0} \sum_{k=1}^{n'} \xi_{i,k}}{(\sum_{k=0}^{n'} \xi_{i,k})^2} > 0,$$

g is also an increasing function.

Let us consider the case $f_0 \in [0, \hat{f}]$. If $f_k \leq \hat{f}$, $g(f_k) \geq f_k$ and $g(f_k) \leq g(\hat{f}) = \hat{f}$. As $g(f_k) = f_{k+1}$, $(f_k)_{k \in \mathbb{N}}$ is an increasing sequence bounded from above by \hat{f} : it converges therefore in $[f_0, \hat{f}]$. Because g is continuous and \hat{f} is the only fixed point in this interval, $(f_k)_{k \in \mathbb{N}}$ tends to \hat{f} .

Similarly, if $f_0 \in [\hat{f}, 1]$, $(f_k)_{k \in \mathbb{N}}$ is a decreasing sequence converging to \hat{f} .

5.2. One-to-one case

All what was said for the several-to-one case still holds in the one-to-one case. Incidentally, as the former is computationally much simpler than the latter, it is a good idea to compute first $\hat{\mathbf{x}}_{s:o}$ and the probabilities $\hat{P}_{s:o}(A_{i,j} \mid C \cap C')$: as $\hat{f}_{s:o}/n' > \hat{f}'_{s:o}/n$ and $\hat{f}_{o:o}/n' = \hat{f}'_{o:o}/n$, the several-to-one assumption is probably correct if $\hat{f}_{s:o}/n' \gg \hat{f}'_{s:o}/n$; and if not, one may first test the one-to-several (subscript “o:s” hereafter) assumption, i.e. reverse the roles of K and K' in all the formulae of Sect. 3, and adopt it if $\hat{f}_{o:s}/n' \ll \hat{f}'_{o:s}/n$.

Ideally, one would compare the likelihood of each assumption and adopt the most likely one. While $\hat{L}_{s:o}$ and $\hat{L}_{o:s}$ are easily computed, no convenient expression was found for $\hat{L}_{o:o}$. However, if $\ln \hat{L}_{s:o}$ and $\ln \hat{L}_{o:s}$ are of the same order, this provides some hint that the one-to-one case (or maybe the several-to-several one!) should be considered. Even then, $\hat{\mathbf{x}}_{s:o}$ will still be a good starting point to find $\hat{\mathbf{x}}_{o:o}$ and there will be no need to compute $\hat{P}_{o:o}(A_{i,j} \mid C \cap C')$ for all couples (i, j) such that $\hat{P}_{s:o}(A_{i,j} \mid C \cap C') \approx \hat{P}_{o:s}(A_{i,j} \mid C \cap C') \approx 1$.

The results of Sect. 4.2 are given in terms of $P_{o:o}(A_{i,j} \mid C \cap C')$. The only difficulty is to estimate this probability from Eq. (40). Because of the combinatorial explosion of the number of terms, an exact computation is hopeless. An approximate value might however be obtained in the following way.

For any M_i , let ϕ be a permutation on K ordering the elements $M_{\phi(1)}, M_{\phi(2)}, \dots, M_{\phi(n)}$ by increasing angular distance to M_i . For $j = 0$ or M'_j in the neighborhood of M_i , and for any $\ell \in \llbracket 1, n \rrbracket$, define

$$P_\ell(A_{i,j} \mid C \cap C') \equiv \frac{\zeta_{i,j} \sum_{j_2=0}^{n'} \dots \sum_{j_\ell=0}^{n'} \prod_{k=2}^\ell \eta_{k,j_k}^{\phi,*}}{\sum_{j_1 \notin J_0^\phi}^{n'} \sum_{j_2=0}^{n'} \dots \sum_{j_\ell=0}^{n'} \prod_{k=1}^\ell \eta_{k,j_k}^\phi}, \quad (45)$$

where $J_1^{\phi,*} \equiv \{j\} \setminus \{0\}$, $J_k^{\phi,*} \equiv (J_{k-1}^{\phi,*} \cup \{j_k\}) \setminus \{0\}$ for all $k \in \llbracket 2, n \rrbracket$, $J_k^\phi \equiv J_k$ for all k ,

$$\eta_{k,j_k}^\phi \equiv \frac{f \xi_{\phi(k),j_k}}{n' - \#J_{k-1}^\phi} \quad \text{and} \quad \eta_{k,j_k}^{\phi,*} \equiv \frac{f \xi_{\phi(k),j_k}}{n' - \#J_{k-1}^{\phi,*}} \quad \text{if } j_k > 0,$$

and $\eta_{k,0}^\phi \equiv \eta_{k,0}^{\phi,*} \equiv \zeta_{\phi(k),0}$.

As $\phi(1) = i$, $P_1(A_{i,j} \mid C \cap C') = P_{s:o}(A_{i,j} \mid C \cap C')$ (cf. Eq. (12)): at first order, we obtain the same result as in the several-to-one case. Since the influence of other K -sources on the result decreases very fast with their angular distance to M_i and M'_j if M_i and M'_j are close to each other, $P_\ell(A_{i,j} \mid C \cap C')$ should rapidly converge to $P_n(A_{i,j} \mid C \cap C') = P_{o:o}(A_{i,j} \mid C \cap C')$, even for small values of ℓ .

Because of the recursive sums in Eq. (45), the computation must in practice be further restricted to sources M'_k in the neighborhood of M_i and M'_j , as explained in Sect. 5.1.1.

Appendix A: Covariance matrix

Let us first remind a few standard results. The probability that a q -dimensional normally distributed random vector \mathbf{W} of mean $\boldsymbol{\mu}$ falls in some domain Ω is

$$P(\mathbf{W} \in \Omega) = \int_{\mathbf{w} \in \Omega} \frac{\exp\left(-\frac{1}{2} [\mathbf{w} - \boldsymbol{\mu}]_B^\top \cdot \Gamma_B^{-1} \cdot [\mathbf{w} - \boldsymbol{\mu}]_B\right)}{(2\pi)^{q/2} (\det \Gamma_B)^{1/2}} d^q \mathbf{w}_B,$$

where $B \equiv (\mathbf{u}_1, \dots, \mathbf{u}_q)$ is a basis, $\mathbf{w}_B \equiv (w_1, \dots, w_q)^\top$ is the column vector in B of $\mathbf{w} = \sum_{i=1}^q w_i \mathbf{u}_i$, $d^q \mathbf{w}_B \equiv dw_1 \times \dots \times dw_q$ and Γ_B is the covariance matrix of \mathbf{W} in B . We note this $\mathbf{W}_B \sim G_q(\boldsymbol{\mu}_B, \Gamma_B)$.

In another basis $B' \equiv (\mathbf{u}'_1, \dots, \mathbf{u}'_q)$, one has $\mathbf{w}_B = T_{B \rightarrow B'} \cdot \mathbf{w}_{B'}$, where $T_{B \rightarrow B'}$ is the transformation matrix from B to B' (i.e. $\mathbf{u}'_j = \sum_{i=1}^q (T_{B \rightarrow B'})_{i,j} \mathbf{u}_i$). Since $d^q \mathbf{w}_B = |\det T_{B \rightarrow B'}| d^q \mathbf{w}_{B'}$ and

$$(\mathbf{w} - \boldsymbol{\mu})_B^\top \cdot \Gamma_B^{-1} \cdot (\mathbf{w} - \boldsymbol{\mu})_B = (\mathbf{w} - \boldsymbol{\mu})_{B'}^\top \cdot \left(T_{B \rightarrow B'}^{-1} \cdot \Gamma_B \cdot [T_{B \rightarrow B'}^{-1}]^\top\right)^{-1} \cdot (\mathbf{w} - \boldsymbol{\mu})_{B'},$$

one still obtains

$$P(\mathbf{W} \in \Omega) = \int_{\mathbf{w} \in \Omega} \frac{\exp\left(-\frac{1}{2} [\mathbf{w} - \boldsymbol{\mu}]_{B'}^\top \cdot \Gamma_{B'}^{-1} \cdot [\mathbf{w} - \boldsymbol{\mu}]_{B'}\right)}{(2\pi)^{q/2} (\det \Gamma_{B'})^{1/2}} d^q \mathbf{w}_{B'},$$

where $\Gamma_{B'} = T_{B \rightarrow B'}^{-1} \cdot \Gamma_B \cdot (T_{B \rightarrow B'}^{-1})^\top$ is the covariance matrix of \mathbf{W} in B' . In the following, B and B' are orthonormal bases, so $T_{B \rightarrow B'}$ is a rotation matrix. From $T_{B \rightarrow B'}^\top = T_{B \rightarrow B'}^{-1}$, one gets $\Gamma_{B'} = T_{B \rightarrow B'}^\top \cdot \Gamma_B \cdot T_{B \rightarrow B'}$.

In a common basis, for independent random vectors $\mathbf{W}_1 \sim G_q(\boldsymbol{\mu}_1, \Gamma_1)$ and $\mathbf{W}_2 \sim G_q(\boldsymbol{\mu}_2, \Gamma_2)$, we have

$$\mathbf{W}_1 \pm \mathbf{W}_2 \sim G_q(\boldsymbol{\mu}_1 \pm \boldsymbol{\mu}_2, \Gamma_1 + \Gamma_2).$$

We now use these results to obtain the covariance matrix of vector $\mathbf{r}_{i,j} \equiv \mathbf{r}'_j - \mathbf{r}_i$, where \mathbf{r}_i and \mathbf{r}'_j are, respectively, the observed positions of source M_i of K and of its counterpart M'_j in K' . We note \mathbf{r}_i^0 and \mathbf{r}'_j^0 their true positions. One has

$$\mathbf{r}_{i,j} = (\mathbf{r}'_j - \mathbf{r}'_j^0) + (\mathbf{r}'_j^0 - \mathbf{r}_i^0) + (\mathbf{r}_i^0 - \mathbf{r}_i).$$

We drop the subscript and the “prime” symbol in the following whenever an expression depends on either M_i or M'_j only.

Let $(\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z)$ be a direct orthonormal basis, with \mathbf{u}_z oriented from the Earth’s center O to the North Celestial Pole and \mathbf{u}_x from O to the Vernal Point. At a point M of right ascension α and declination δ , a direct orthonormal basis $(\mathbf{u}_r, \mathbf{u}_\alpha, \mathbf{u}_\delta)$ is defined by

$$\begin{aligned} \mathbf{u}_r &\equiv \frac{\mathbf{OM}}{\|\mathbf{OM}\|} = \cos \delta \cos \alpha \mathbf{u}_x + \cos \delta \sin \alpha \mathbf{u}_y + \sin \delta \mathbf{u}_z, \\ \mathbf{u}_\alpha &\equiv \frac{\partial \mathbf{u}_r / \partial \alpha}{\|\partial \mathbf{u}_r / \partial \alpha\|} = -\sin \alpha \mathbf{u}_x + \cos \alpha \mathbf{u}_y, \\ \mathbf{u}_\delta &\equiv \frac{\partial \mathbf{u}_r / \partial \delta}{\|\partial \mathbf{u}_r / \partial \delta\|} = -\sin \delta \cos \alpha \mathbf{u}_x - \sin \delta \sin \alpha \mathbf{u}_y + \cos \delta \mathbf{u}_z. \end{aligned}$$

The uncertainty ellipse on the position of M is characterized by the lengths a and b of the semi-major and semi-minor axes, and by the position angle β between the North and the semi-major axis. Let \mathbf{u}_a and \mathbf{u}_b be unit vectors directed respectively along the major and the minor axes, and such that $(\mathbf{u}_r, \mathbf{u}_a, \mathbf{u}_b)$ is a direct orthonormal basis and $\beta \equiv (\mathbf{u}_\delta, \mathbf{u}_a)$ is in $[0, \pi]$ when counted eastward. In the plane oriented by $+\mathbf{u}_r$,

$$T_{(\mathbf{u}_a, \mathbf{u}_b) \rightarrow (\mathbf{u}_\alpha, \mathbf{u}_\delta)} = \begin{pmatrix} \sin \beta & \cos \beta \\ -\cos \beta & \sin \beta \end{pmatrix} \equiv \text{Rot}(\beta),$$

since $(\mathbf{u}_\alpha, \mathbf{u}_\delta)$ is obtained from $(\mathbf{u}_a, \mathbf{u}_b)$ by a $(\beta - \pi/2)$ -counterclockwise rotation. As³

$$\Gamma_{(\mathbf{u}_a, \mathbf{u}_b)} = \begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix} \equiv \text{Diag}(a^2, b^2),$$

one has $\Gamma_{(\mathbf{u}_\alpha, \mathbf{u}_\delta)} = \text{Rot}^\top(\beta) \cdot \text{Diag}(a^2, b^2) \cdot \text{Rot}(\beta)$.

As noticed by Pineau et al. (2011), for sources close to the Poles, $(\mathbf{u}_{\alpha_i}, \mathbf{u}_{\delta_i}) \neq (\mathbf{u}_{\alpha'_j}, \mathbf{u}_{\delta'_j})$, so one needs to define a common basis. We use the same basis as them, noted (\mathbf{t}, \mathbf{n}) below. While the results we get are intrinsically the same, some people may find our expressions more convenient.

Denote $\psi \equiv (\widehat{\mathbf{u}_{r_i}, \mathbf{u}_{r'_j}}) \in [0, \pi]$ the angular distance between M_i and M'_j , and $\mathbf{n} \equiv \mathbf{u}_{r_i} \times \mathbf{u}_{r'_j} / \|\mathbf{u}_{r_i} \times \mathbf{u}_{r'_j}\|$ a unit vector perpendicular to the plane (O, M_i, M'_j) . One has $\mathbf{u}_{r_i} \cdot \mathbf{u}_{r'_j} = \cos \psi$, so

$$\psi = \arccos(\cos \delta_i \cos \delta'_j \cos[\alpha'_j - \alpha_i] + \sin \delta_i \sin \delta'_j), \quad (\text{A.1})$$

and $\|\mathbf{u}_{r_i} \times \mathbf{u}_{r'_j}\| = \sin \psi$.

Let $\gamma_i \equiv (\widehat{\mathbf{n}, \mathbf{u}_{\delta_i}})$ and $\gamma'_j \equiv (\widehat{\mathbf{n}, \mathbf{u}_{\delta'_j}})$ be angles oriented clockwise around $+\mathbf{u}_{r_i}$ and $+\mathbf{u}_{r'_j}$, respectively. Angle γ_i is fully determined by following expressions:

$$\begin{aligned} \cos \gamma_i &= \mathbf{n} \cdot \mathbf{u}_{\delta_i} = \frac{1}{\sin \psi} (\mathbf{u}_{r_i} \times \mathbf{u}_{r'_j}) \cdot \mathbf{u}_{\delta_i} = \frac{1}{\sin \psi} (\mathbf{u}_{\delta_i} \times \mathbf{u}_{r_i}) \cdot \mathbf{u}_{r'_j} = \frac{1}{\sin \psi} \mathbf{u}_{\alpha_i} \cdot \mathbf{u}_{r'_j} \\ &= \frac{\cos \delta'_j \sin(\alpha'_j - \alpha_i)}{\sin \psi}; \\ \sin \gamma_i &= -\mathbf{n} \cdot \mathbf{u}_{\alpha_i} = -\frac{1}{\sin \psi} (\mathbf{u}_{r_i} \times \mathbf{u}_{r'_j}) \cdot \mathbf{u}_{\alpha_i} = -\frac{1}{\sin \psi} (\mathbf{u}_{\alpha_i} \times \mathbf{u}_{r_i}) \cdot \mathbf{u}_{r'_j} = \frac{1}{\sin \psi} \mathbf{u}_{\delta_i} \cdot \mathbf{u}_{r'_j} \\ &= \frac{\cos \delta_i \sin \delta'_j - \sin \delta_i \cos \delta'_j \cos(\alpha'_j - \alpha_i)}{\sin \psi}. \end{aligned}$$

³ We seize this opportunity to correct equations (A.8) to (A.11) of Pineau et al. (2011): a and b should be replaced by their squares in these formulae.

Similarly,

$$\cos \gamma'_j = \frac{\cos \delta_i \sin(\alpha'_j - \alpha_i)}{\sin \psi} \quad \text{and} \quad \sin \gamma'_j = \frac{\cos \delta_i \sin \delta'_j \cos(\alpha'_j - \alpha_i) - \sin \delta_i \cos \delta'_j}{\sin \psi}.$$

Note that determining γ_i and γ'_j themselves might slow down the computations: for instance, only the sines and cosines of β_i and γ_i are of interest in the matrices $\text{Rot}(\beta_i + \gamma_i)$ used hereafter, as is obvious from the expansion of $\sin(\beta_i + \gamma_i)$ and $\cos(\beta_i + \gamma_i)$. The same holds for $\text{Rot}(\beta'_j + \gamma'_j)$ and other matrices.

Let $\mathbf{t} \equiv \mathbf{n} \times \mathbf{u}_r$: \mathbf{t} is a unit vector tangent in M_i to the minor arc of great circle going from M_i to M'_j . Project the sphere on the plane $(M_i, \mathbf{t}, \mathbf{n})$ tangent to the sphere in M_i (which specific projection does not matter since we consider only K' -sources in the neighborhood of M_i): one has $\mathbf{r}_{i,j} \approx \psi \mathbf{t}$, and the basis (\mathbf{t}, \mathbf{n}) is obtained from $(\mathbf{u}_a, \mathbf{u}_b)$ by a $(\beta + \gamma - \pi/2)$ -counterclockwise rotation around $+\mathbf{u}_r$, so, in (\mathbf{t}, \mathbf{n}) ,

$$\Gamma_i = \text{Rot}^T(\beta_i + \gamma_i) \cdot \text{Diag}(a_i^2, b_i^2) \cdot \text{Rot}(\beta_i + \gamma_i) \quad \text{and} \quad \Gamma'_j = \text{Rot}^T(\beta'_j + \gamma'_j) \cdot \text{Diag}(a_j'^2, b_j'^2) \cdot \text{Rot}(\beta'_j + \gamma'_j).$$

As $\mathbf{r}_i \sim G_2(\mathbf{0}, \Gamma_i)$ and $\mathbf{r}'_j \sim G_2(\mathbf{0}, \Gamma'_j)$, one has $\mathbf{r}_{i,j} \sim G_2(\mathbf{0}, \Gamma_{i,j})$ if the true positions are identical, where $\Gamma_{i,j} \equiv \Gamma_i + \Gamma'_j$.

If the positional uncertainty on M_i is unknown, one may assume that $\Gamma_i = \sigma^2 \text{Diag}(1, 1)$, with the same σ for all K -sources, and derive $\hat{\sigma} \equiv \sigma$ by maximizing the likelihood to observe the distribution of K -sources given that of K' -sources (see Sects. 3.2 and 4.2). For a galaxy, however, the positional uncertainty on its center is likely to increase with its size. If the position angle θ_i (counted eastward from the North) and the major and minor diameters D_i and d_i of the best-fitting ellipse of some isophote are known for M_i (for instance, parameters PA, D_{25} and $d_{25} \equiv D_{25}/R_{25}$ taken from the RC3 catalog (de Vaucouleurs et al. 1991) or HyperLeda (Paturel et al. 2003)), one may model Γ_i as

$$\Gamma_i = \text{Rot}^T(\gamma_i + \theta_i) \cdot \text{Diag}(\sigma^2 + [\nu D_i]^2, \sigma^2 + [\nu d_i]^2) \cdot \text{Rot}(\gamma_i + \theta_i) = \sigma^2 \text{Diag}(1, 1) + \nu^2 \text{Rot}^T(\gamma_i + \theta_i) \cdot \text{Diag}(D_i^2, d_i^2) \cdot \text{Rot}(\gamma_i + \theta_i),$$

and derive both $\hat{\sigma} \equiv \sigma$ and $\hat{\nu} \equiv \nu$ from the maximum likelihood. Such a technique might indeed be used to estimate the accuracy of coordinates in some catalog (see Paturel & Petit (1999) for another method).

If the positional uncertainty on M'_j is also unknown, one can put

$$\Gamma'_j = \sigma'^2 \text{Diag}(1, 1) + \nu'^2 \text{Rot}^T(\gamma'_j + \theta'_j) \cdot \text{Diag}(D_j'^2, d_j'^2) \cdot \text{Rot}(\gamma'_j + \theta'_j)$$

with the same σ' and ν' for all K' -sources. As $\gamma'_j + \theta'_j = \gamma_i + \theta_i$, only $\hat{\sigma} \equiv (\sigma^2 + \sigma'^2)^{1/2}$ and $\hat{\nu} \equiv (\nu^2 + \nu'^2)^{1/2}$ may be obtained⁴ from the maximum likelihood, not σ , σ' , ν or ν' .

A similar technique can be applied if the true centers of a source in K and of its counterpart in K' may differ. This might be in particular useful when associating galaxies from an optical catalog and from a ultraviolet or far-infrared catalog, because, while the optical is dominated by smoothly-distributed evolved stellar populations, the ultraviolet and the far-infrared mainly trace star-forming regions. Observations of galaxies by Kuchinski et al. (2000) have indeed shown that galaxies are very patchy in the ultraviolet, and the same has been observed in the far-infrared. As the angular distance between the true centers should increase with the size of the galaxy, one may model this as $\mathbf{r}_i^0 - \mathbf{r}_i^0 \sim G_2(\mathbf{0}, \Gamma_0)$, where $\Gamma_0 = \nu_0^2 \text{Rot}^T(\gamma_i + \theta_i) \cdot \text{Diag}(D_i^2, d_i^2) \cdot \text{Rot}(\gamma_i + \theta_i)$.

In the most general case,

$$\mathbf{r}_{i,j} \sim G_2(\mathbf{0}, \Gamma_{i,j}),$$

with $\Gamma_{i,j} \equiv \Gamma_i + \Gamma'_j + \Gamma_0$. Once again, if σ , σ' , ν , ν' and ν_0 are unknown, the quantities $\hat{\sigma} \equiv (\sigma^2 + \sigma'^2)^{1/2}$ and $\hat{\nu} \equiv (\nu^2 + \nu'^2 + \nu_0^2)^{1/2}$ may be determined as indicated in Sects. 3.2 and 4.2.

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⁴ However, as noticed by de Vaucouleurs & Head (1978) in a different context, if three samples with unknown uncertainties σ_i ($i \in \llbracket 1, 3 \rrbracket$) are available and if the $\sigma_{i,j} \equiv (\sigma_i^2 + \sigma_j^2)^{1/2}$ may be estimated for all the pairs $(i, j)_{j \neq i} \in \llbracket 1, 3 \rrbracket^2$, as in our case, then σ_i may be determined for each sample. Paturel & Petit (1999) used this technique to compute the accuracy of galaxy coordinates.